Density Functional Study of the magnetic structure on spin frustrated MnSb$_2$S$_4$ and Sr$_2$MOsO$_6$ (M = Cu, Ni) CHUAN TIAN, CHANGHOON LEE, ERJUN KAN, North Carolina State University, FANG WU$^1$, Nanjing Forestry University, MIKE WHANGBO, North Carolina State University — We explored the electronic structures of two spin-frustrated magnetic systems monoclinic MnSb$_2$S$_4$ and Sr$_2$MOsO$_6$ (M = Cu, Ni) on the basis of first principles DFT calculations. The spin exchanges of MnSb$_2$S$_4$ are frustrated within each MnS$_4$ chain and between adjacent MnS$_4$ chains, which explains the observed helical spin order of MnSb$_2$S$_4$. We predict that MnSb$_2$S$_4$ is multiferroic with ferroelectric polarization of $\sim$14 $\mu$C/m$^2$ along the chain direction, and a field-induced reversal of the ferroelectric polarization occurs by reversing the direction of the helical spin rotation. The ordered double perovskites Sr$_2$MOsO$_6$ (M = Cu, Ni), reported to be half-metallic, are found to be magnetic insulators. The magnetic structures of Sr$_2$MOsO$_6$ were probed by evaluating their spin exchanges.

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